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A NEW APPROACH TO PREDICT OPTIMAL SALINITIES FOR SURFACTANT FORMULATIONS

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The continous development of improved oil recovery (IOR) techniques pushes the limits in terms of oil extraction capabilities. Among these techniques, the enhanced oil recovery (EOR) techniques, and more precisely the chemical EOR (cEOR) has been the focus of a renewed interest from oil companies. The cEOR consists in the injection of combinations of alkaline/surfactants/polymer (ASP) to mobilize oil trapped in reservoir, by acting on capillary forces. One of the key properties in cEOR is the optimal salinity (S*) of brine/surfactant/oil systems. Each reservoir has specific characteristics (pressure, temperature, oil composition, brine composition and hardness…), and thus the conception of a well adapted ASP formulation is a time-consuming task.

We early proposed the use of the chemoinformatics to develop efficient tools for fast and accurate estimation of surfactant optimal salinities [1-2]. We have previously demonstrated the robustness of models based on support vector machine (SVM) and molecular descriptors such as substructural molecular fragments (SMF). However, quantitative structure property relationship (QSPR) based models we developed possess their intrinsic limitations, for instance they do not account for the diversity of reservoir characteristics.

We recently supplement our database with additional experimental data, including new families of surfactants (alkylbenzene sulfonate, ABS), a wider range of temperatures ($20 < T < 120$ °C), n-alkanes from nC_8 to nC_{18}, and various brine composition and hardness. To overcome artefacts due to the database content, we investigated the use of an empirical S* model that could be fed with values predicted using SVM based models. The exploration of the SVM kernel parmeters (epsilon, cost, gamma) matrix can be costly in terms of computational resources. Thus, a new approach is proposed to select best SVM kernel parmeters with the help of an optimization library developed at IFP Energies nouvelles. The optimization of SVM kernel parameters including a double cross-validation procedure now only necessitates few minutes. The accuracy of the new approach (empirical model feed with QSPR predictions) is then evaluated performing comparisons between predicted and experimental data.

1. Moreau P. et al. *SPE International Symposium on Oilfield Chemistry*, 2013, 164091-MS.
2. Muller C. et al. *Energy Fuels*, 2015, **29 (7)**: 4281–4288.